

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
 Data File : BF140431.D
 Acq On : 16 Nov 2024 15:49
 Operator : RC/JU
 Sample : P4821-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BP-F-24

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140431.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	6	14	rVB	943458	1336814	42.77%	5.980%
2	5.092	499	510	526	rVB	43346	74046	2.37%	0.331%
3	5.504	574	580	595	rBV	1974916	2609451	83.49%	11.673%
4	6.510	745	751	768	rVB	2015715	2729269	87.32%	12.209%
5	6.875	807	813	818	rBV	510765	652938	20.89%	2.921%
6	7.434	902	908	913	rBV	1330987	1725506	55.21%	7.719%
7	7.681	943	950	962	rBV	35623	55771	1.78%	0.249%
8	8.151	1025	1030	1047	rBV	646811	836572	26.77%	3.742%
9	9.228	1207	1213	1223	rBV	2434127	3125540	100.00%	13.982%
10	9.910	1323	1329	1338	rBV	709017	925490	29.61%	4.140%
11	10.622	1444	1450	1458	rBV	505217	634769	20.31%	2.840%
12	10.698	1458	1463	1478	rBV	1478387	1923761	61.55%	8.606%
13	10.927	1494	1502	1513	rBV	74942	108408	3.47%	0.485%
14	11.398	1576	1582	1590	rBV	759346	981797	31.41%	4.392%
15	11.463	1590	1593	1597	rVB2	26450	31899	1.02%	0.143%
16	11.921	1666	1671	1685	rBV	275768	464644	14.87%	2.079%
17	12.421	1751	1756	1760	rBV	22783	36074	1.15%	0.161%
18	12.710	1801	1805	1811	rBV2	24244	49653	1.59%	0.222%
19	12.980	1846	1851	1859	rBV	2077961	2708680	86.66%	12.117%
20	14.039	2027	2031	2040	rVB	485321	658933	21.08%	2.948%
21	15.539	2280	2286	2295	rVB	419687	684318	21.89%	3.061%

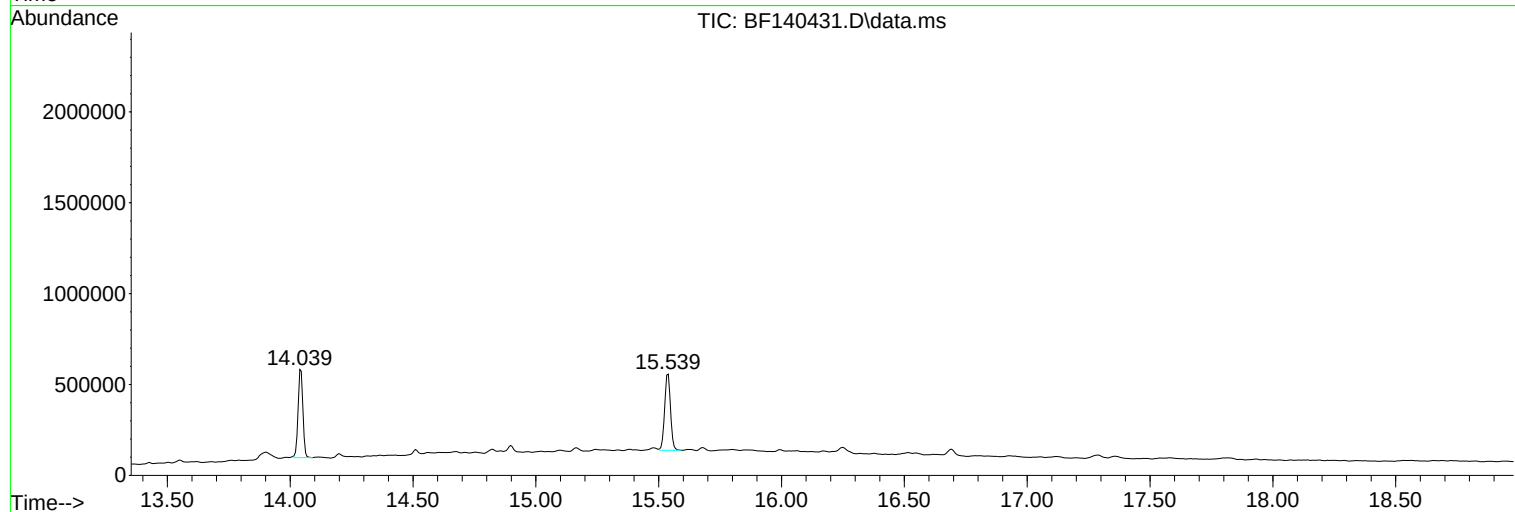
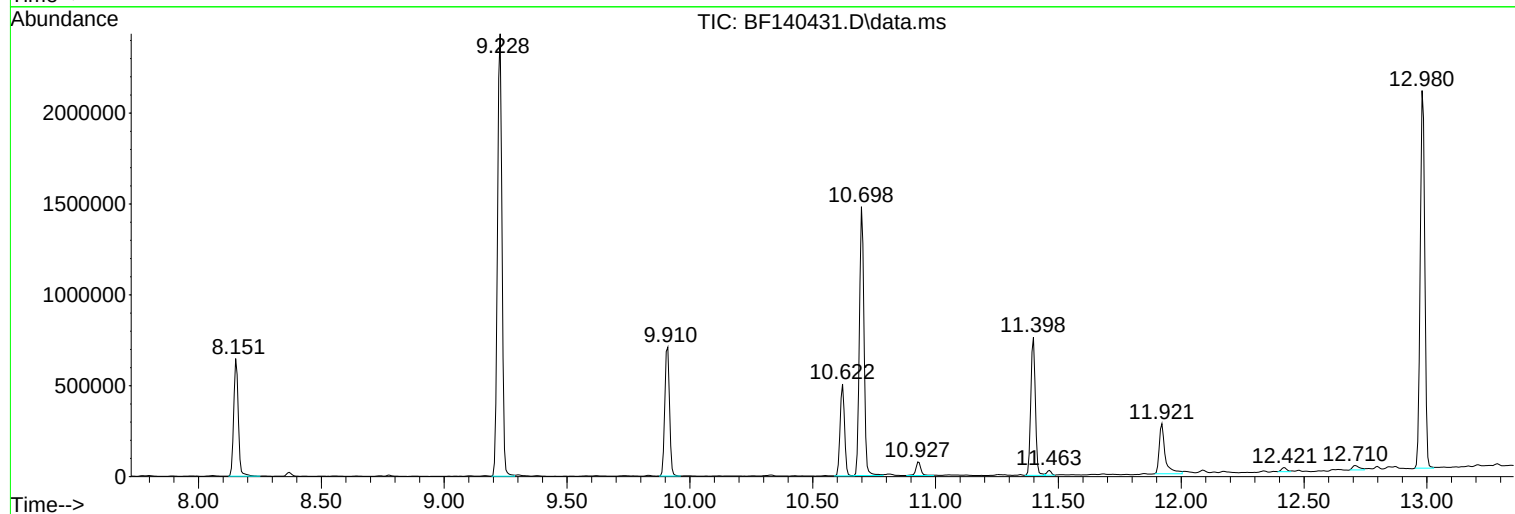
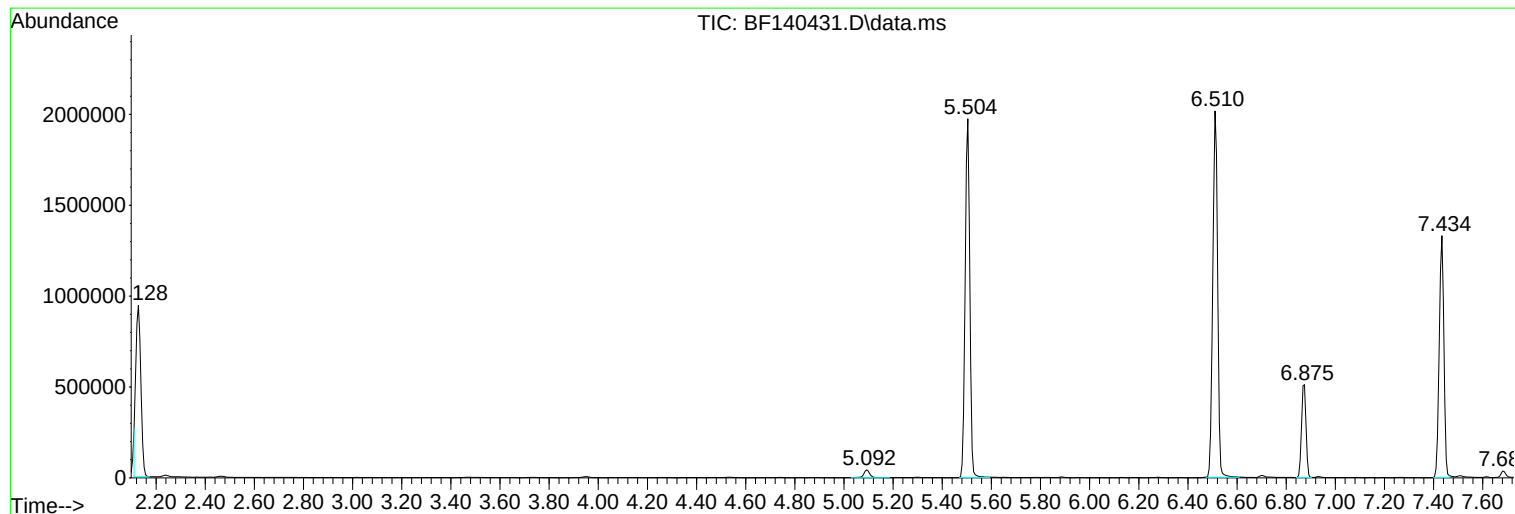
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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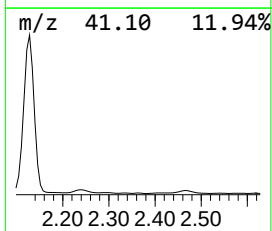
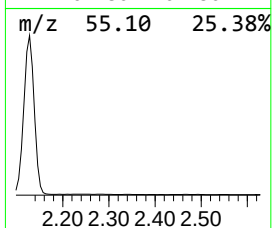
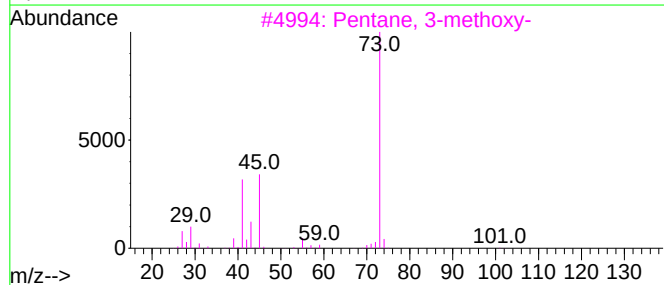
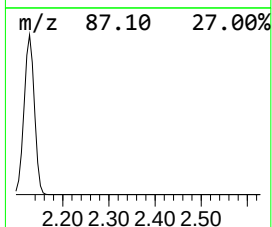
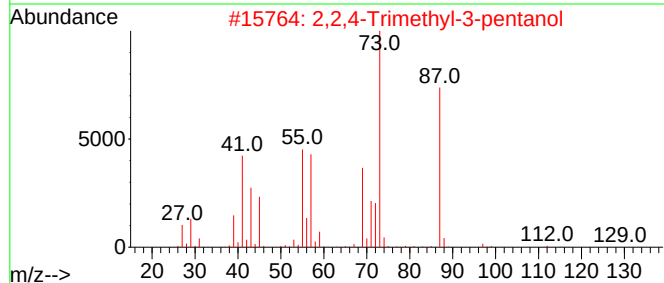
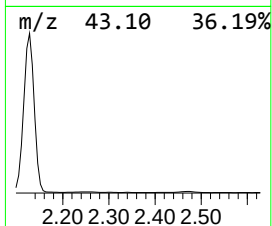
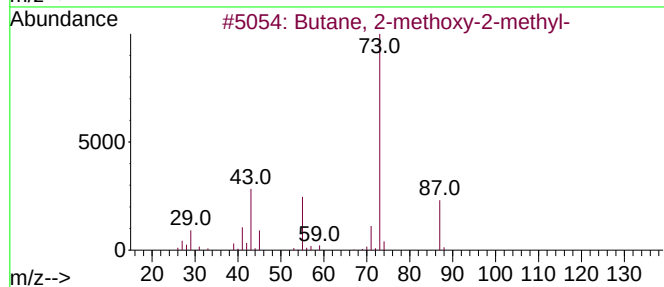
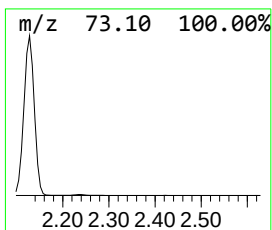
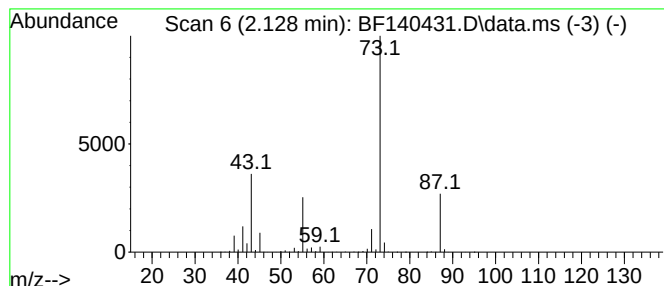
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	40.95 ng	1336810	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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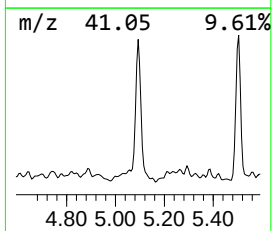
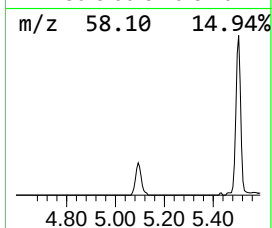
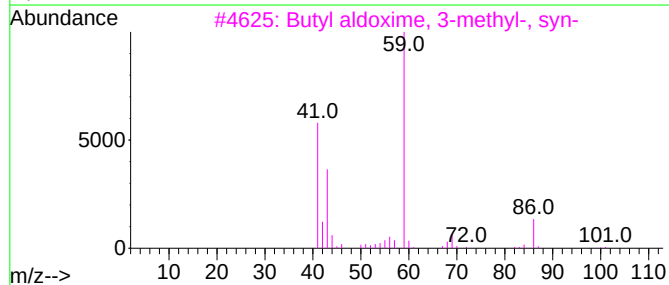
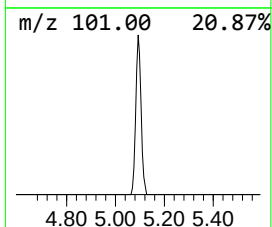
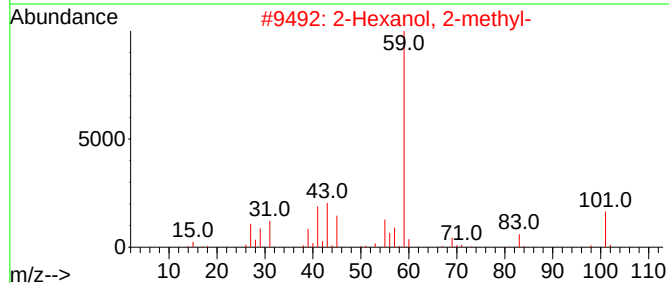
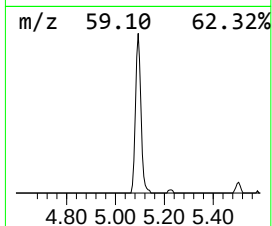
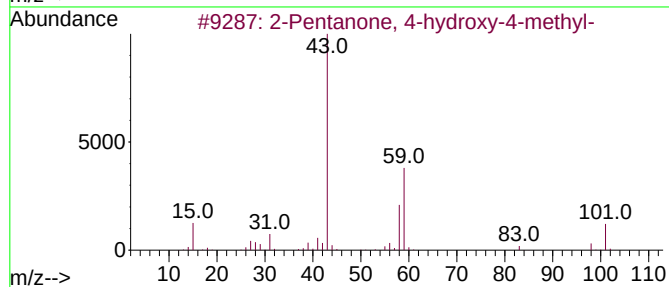
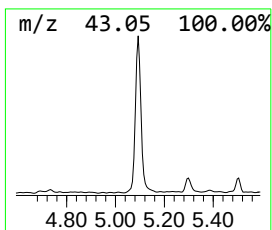
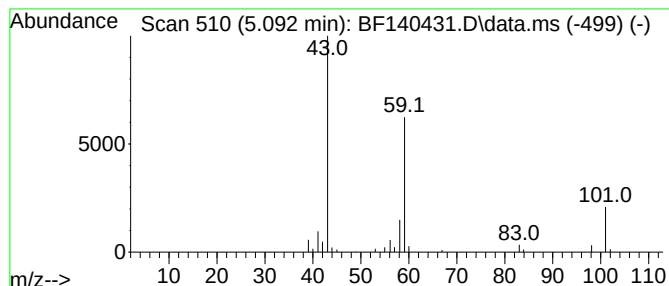
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	2.27 ng	74046	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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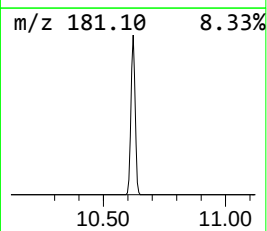
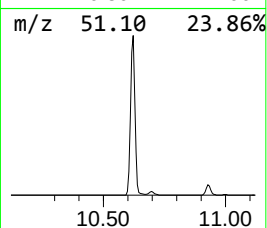
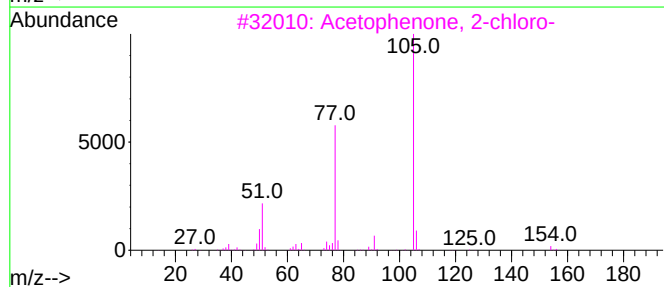
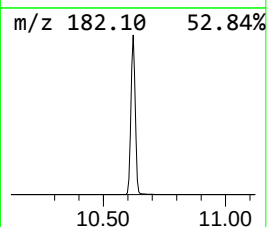
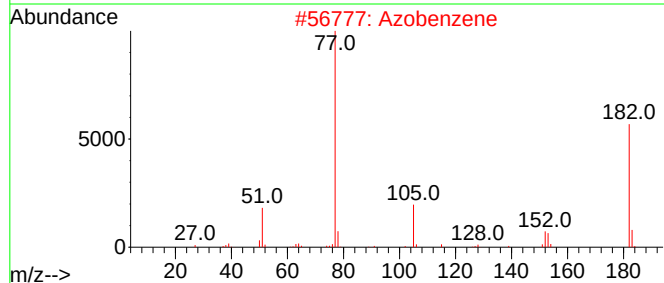
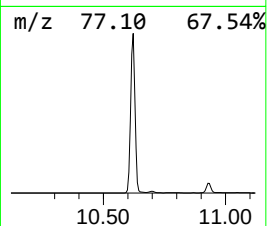
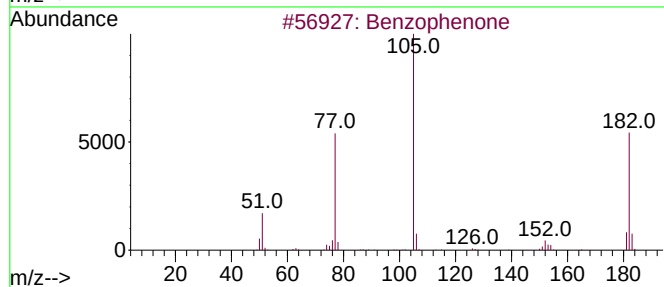
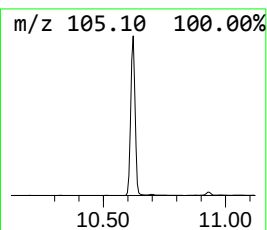
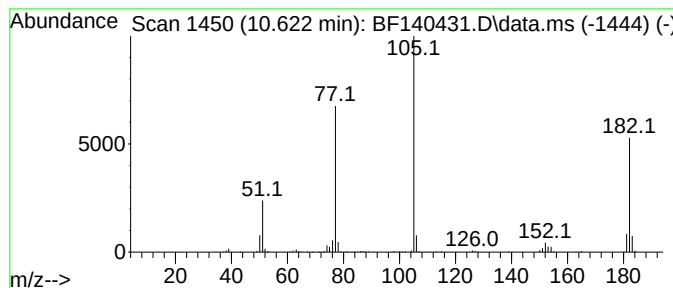
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.621	13.72 ng	634769	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	72
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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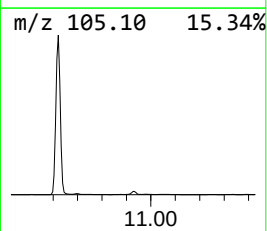
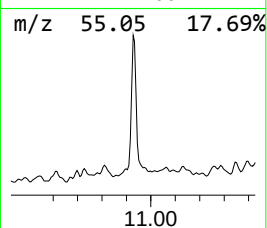
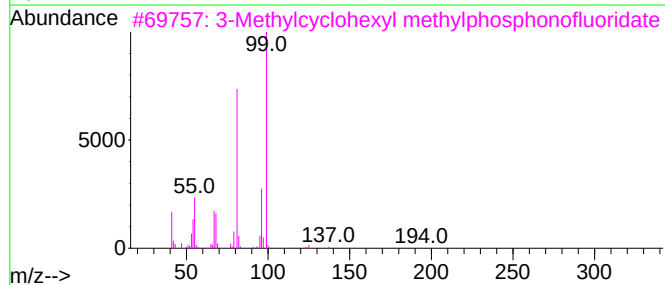
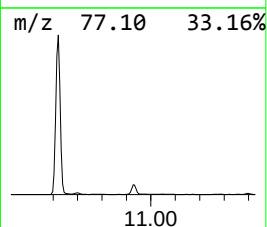
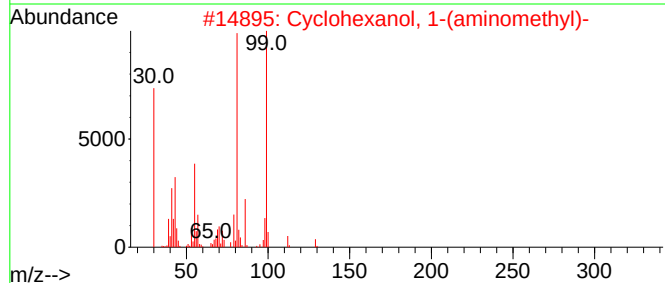
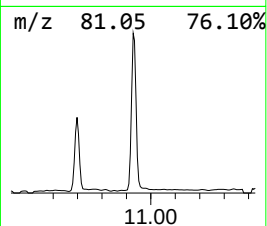
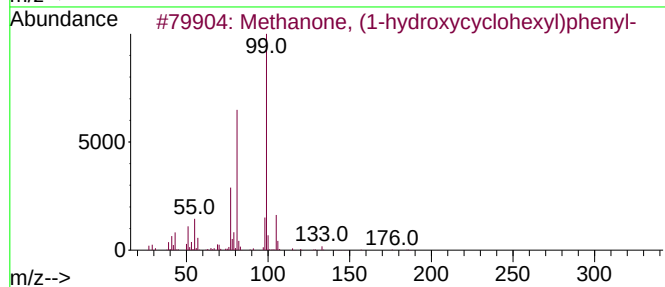
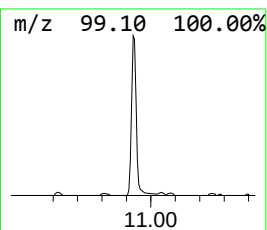
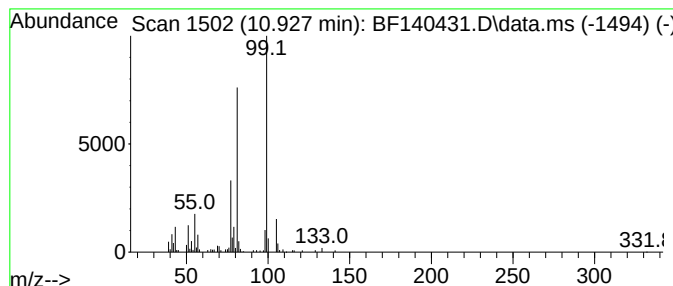
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Peak Number 4 Methanone, (1-hydroxycyclohexyl) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.927	2.21 ng	108408	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	64
2			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	50
3			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	38
4			3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	25
5			1-(Prop-2-yn-1-yl)cyclohexyl car...	181	C10H15NO2	000358-52-1	23



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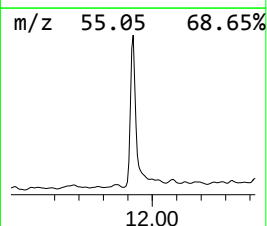
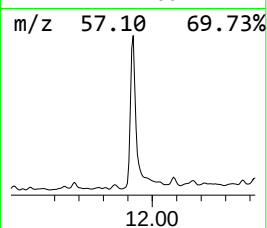
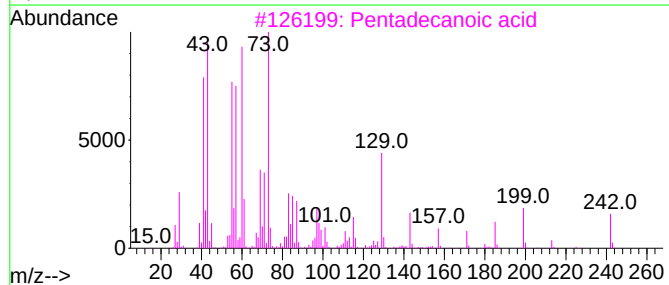
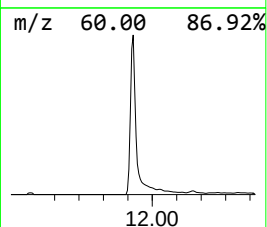
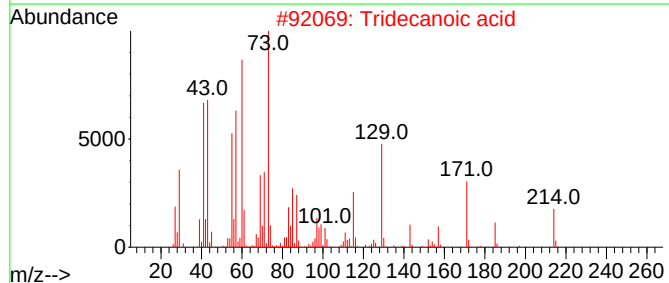
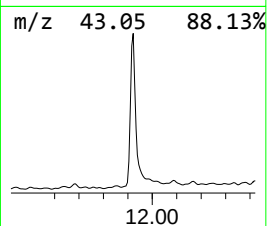
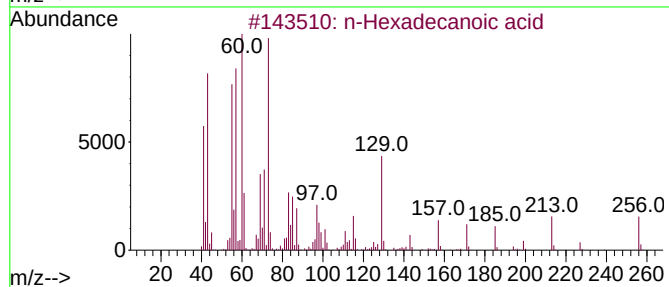
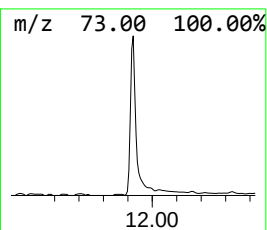
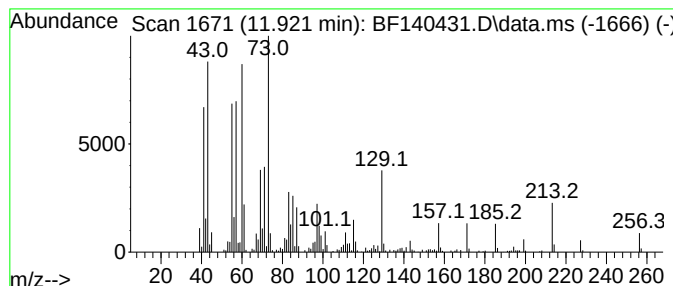
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	9.47 ng	464644	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.128	41.0	ng	1336810	1	6.875	652938	20.0
2-Pentanone, 4-...	5.092	2.3	ng	74046	1	6.875	652938	20.0
Benzophenone	10.621	13.7	ng	634769	3	9.910	925490	20.0
Methanone, (1-h...	10.927	2.2	ng	108408	4	11.398	981797	20.0
n-Hexadecanoic ...	11.922	9.5	ng	464644	4	11.398	981797	20.0